

Trifluoromethanesulfonic acid
1493-13-6 | DTXSID2044397

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.32 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.59e-01

Confidence level: 6.77e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methanesulfonic acid</div> <div>Measured: 10.4</div> <div>Predicted: 6.76</div>	<div>Image not found</div> <div>Methylarsonic acid</div> <div>Measured: 1.83</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>Monosodium methanearsonate</div> <div>Measured: 3.58</div> <div>Predicted: N/A</div>
<div>Image not found</div> <div>2-Hydroxyethanesulfonic acid</div> <div>Measured: 7.93</div> <div>Predicted: 6.22</div>	<div>Image not found</div> <div>L-Taurine</div> <div>Measured: 6.45e-01</div> <div>Predicted: 8.59e-01</div>	